

1,4-Dioxane
123-91-1 | DTXSID4020533

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 103 °C

Global applicability domain: Inside

Local applicability domain index: 8.75e-01

Confidence level: 7.69e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,4-Dioxane</div> <div>Measured: 102</div> <div>Predicted: 103</div>	<div>Image not found</div> <div>1,3-Dioxane</div> <div>Measured: 106</div> <div>Predicted: 103</div>	<div>Image not found</div> <div>Methyl glycidyl ether</div> <div>Measured: 113</div> <div>Predicted: 101</div>
<div>Image not found</div> <div>2-Methyl-1,3-dioxolane</div> <div>Measured: 81.5</div> <div>Predicted: 99.9</div>	<div>Image not found</div> <div>Chloromethyl acetate</div> <div>Measured: 116</div> <div>Predicted: 116</div>	